

Path Integral Monte-Carlo Calculations for Relativistic Oscillator

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Abstract

The problem of Relativistic Oscillator has been studied in the framework of Path Integral Monte-Carlo(PIMC) approach. Ultra-relativistic and non-relativistic limits have been discussed. We show that PIMC method can be effectively used for investigation of relativistic systems.

1 Introduction

Path Integral Monte-Carlo method [1] is one of the most popular *ab initio* numerical approach of the investigation of quantum systems. Especially this method becomes useful for modelling properties of quantum problems of many bodies in case the Schrodinger Equations become difficult to study but the number of quantum degrees of freedom is still not so large for using Quantum Statistics.

This work is devoted to the generalization of Path Integral Monte Carlo in case of the relativistic systems. There are many physical problems connected with simulations of relativistic quantum mechanical systems. Relativistic corrections play very essential role in physics of the atomic systems with heavy elements due to the strong interaction potentials. One may find the problems with simulations of relativistic quantum systems in the nuclear physics, physics of hadron structure and quark-gluon plasma, in relativistic astrophysics. Recently an another interesting application of the relativistic quantum mechanics has arisen. These are so called (Pseudo) Relativistic Condensed Matter systems and one of the most famous examples of such systems is Graphene [2].

The remarkable property of Graphene is that it's effective charge excitations have very small mass (in case of the idealistic graphene without defects and boundary effects the mass of excitations is equal to zero). On the other hand, the interaction between excitations is very strong. It means that the excitations on the graphene sheet can be treated as some strongly interacted two-dimensional relativistic gas with instantaneous interaction.

The correct formulation of the many-body relativistic quantum-mechanical problem has some well-known difficulties. The kinetic and potential part of the Hamiltonian must be invariant at Lorentz transformation. The kinetic part of Hamiltonian can be formulated

in Lorentz-invariant form relatively easy but relativistic formulation of interaction requires the quantum field theory approach in general case. If we want to work in the framework of the quantum mechanics approach we are to use some additional assumptions. In this work we study just kinetic part of Hamiltonian. The interaction part can not be studied in general case. For the first approximation let us consider the relativistic quantum systems with instantaneous interaction between particles. This approximation works very well in case of Relativistic Quantum Chemistry and for investigation of the properties (Pseudo) Relativistic Condensed Matter systems like graphene where the correction from relativistic nature of the interaction is fortunately very small in comparison with the correction that comes from relativistic nature of the particles. The nuclear and high-energy systems require some special considerations and these tasks will be the key point of our future works.

Relativistic generalization of the Path Integral approach for quantum mechanical systems has a long history [3], [4]. Today this approach is becoming more and more popular and find its application in high-energy physics [5], [6]. Now we briefly discuss the main statements of Path Integral formalism for relativistic quantum-mechanical system.

2 Oscillator

Simple harmonic oscillator has a hamiltonian function

$$H = m + \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2, \quad (1)$$

where $V(q) = \frac{1}{2}m\omega^2 q^2$ - potential energy, $T(p) = \frac{p^2}{2m}$ - kinetic energy and m - rest mass. The expression $\frac{p^2}{2m}$ is kinetic energy in non-relativistic case. Generalization of kinetic energy is $T(p) = \sqrt{p^2 + m^2}$. So the generalization of simple harmonic oscillator is the following

$$H = \sqrt{p^2 + m^2} + \frac{1}{2}m\omega^2 q^2. \quad (2)$$

In this work we want to calculate the system with hamiltonian function (2) by Path Integral Monte-Carlo(PIMC) Metropolis algorithm, but at first, this method should be generalized for relativistic case. To compare the results we have used two limits of this hamiltonian function, in which we have analytical expressions for observables:

$$m^2 \gg p^2 \text{ (Non-relativistic limit)} \quad (3)$$

$$m^2 \ll p^2 \text{ (Ultra-relativistic limit)} \quad (4)$$

There are only two dimensional parameters m and ω , as we will see later, conditions (3) and (4) can be overwrite in terms of m and ω .

2.1 Non-relativistic limit

In this section the limit $m^2 \gg p^2$ is considered. We should understand it in terms of average values, it means that $m^2 \gg \langle p^2 \rangle$. Non-relativistic limit of the kinetic energy from (2) is the

following

$$T(p) = \sqrt{p^2 + m^2} = m(1 + \frac{p^2}{2m^2} + O(\left(\frac{p}{m}\right)^4)) \approx m + \frac{p^2}{2m}$$

and we obtain simple harmonic oscillator.

$$H = m + \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2. \quad (5)$$

The energy and probability density of ground state is well known for this hamiltonian function

$$E_0 = m + \frac{\omega}{2}, \quad (6)$$

$$\rho(q) = |\psi(q)|^2 = \left(\frac{m\omega}{\pi}\right)^{\frac{1}{2}} \exp(-m\omega q^2), \quad (7)$$

where $\psi(q)$ is a wave function of this ground state. The virial theorem gives us relation between kinetic and potential energy

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{1}{2}m\omega^2 q^2 \right\rangle \text{ or } \langle T(p) - m \rangle = \langle V(q) \rangle.$$

Using (5) we obtain

$$\langle T(p) - m \rangle = \frac{1}{2}(E_0 - m) = \langle V(q) \rangle = \frac{\omega}{4}. \quad (8)$$

Correlation function $\langle q(t)q(t+s) \rangle$ for this system is the following

$$\langle q(t)q(t+s) \rangle = \frac{1}{2m\omega} e^{-w|s|}. \quad (9)$$

We have a list of observables (6), (7), (9) to compare results with numerical calculations by PIMC.

We can formulate condition (3) in terms of m and ω , that is necessary to distinguish different limits. Using (3), (8) we can obtain $\langle p^2 \rangle \sim m\omega$ and $m \gg \omega$. It means that we consider heavy particles and soft potential in this case.

2.2 Ultra-relativistic limit

Our next step is a consideration of hamiltonian function (2) in the limit (4). The kinetic energy in this case is the following

$$T(p) = \sqrt{p^2 + m^2} = |p| \left(1 + \frac{m^2}{2p^2} + O\left(\left(\frac{m}{p}\right)^4\right) \right) \approx |p|.$$

That's enough to take only zero order to describe the behavior of the system. We have

$$H = |p| + \frac{1}{2}m\omega^2 q^2. \quad (10)$$

We can solve Shroedinger equation for this hamiltonian function in momentum representation and find energy of ground state and corresponding density of probability

$$E_0 = \lambda_0(m\omega^2)^{1/3}, \quad (11)$$

where $\lambda_0 = 0.808617\dots$,

$$\rho(q) = \frac{\int \int \frac{dp dk}{(2\pi)^2} \text{Ai}\left(\left(\frac{2}{m\omega^2}\right)^{1/3}(|p| - \lambda_0)\right) \text{Ai}\left(\left(\frac{2}{m\omega^2}\right)^{1/3}(|k| - \lambda_0)\right) e^{-i(p-k)q}}{\int \frac{dp}{2\pi} \text{Ai}^2\left(\left(\frac{2}{m\omega^2}\right)^{1/3}(|p| - \lambda_0)\right)}, \quad (12)$$

where $\text{Ai}(x)$ is the Airy function. The virial theorem for this hamiltonian function gives us the relation between kinetic and potential energy

$$\langle T(p) \rangle = 2\langle V(q) \rangle,$$

so we can obtain results for kinetic and potential energy

$$\langle T(p) \rangle = \frac{2\lambda_0}{3}(m\omega^2)^{1/3}, \quad (13)$$

$$\langle V(q) \rangle = \frac{\lambda_0}{3}(m\omega^2)^{1/3}, \quad (14)$$

$$\langle q^2 \rangle = \frac{2\lambda_0}{3(m\omega^2)^{2/3}}. \quad (15)$$

Using the virial theorem, we have $\langle |p| \rangle \sim (m\omega^2)^{1/3}$. Let's suggest $\langle |p| \rangle^2 \sim \langle p^2 \rangle$, than we can obtain ratio

$$\frac{m^2}{\langle p^2 \rangle} \sim \left(\frac{m}{\omega}\right)^{4/3} \ll 1.$$

For ultra-relativistic case we have the opposite expression for mass and frequency

$$\omega \gg m.$$

We have obtained one more list of observables for comparison with PIMC calculations.

3 Density matrix for Monte-Carlo calculations

In this section we consider quantum mechanics system at finite temperature. One can find the full consideration of this question in [1]. Average value of some operator A

$$\langle A \rangle = \frac{\text{tr}(Ae^{-\beta H})}{\text{tr}(e^{-\beta H})},$$

where operator $e^{-\beta H}$ is the density matrix and $\beta = 1/\theta$ is inverse temperature of the system to be considered. For PIMC method we should consider zero temperature limit. Matrix element of density matrix in coordinate representation is

$$\rho(q, q'; \beta) = \langle q | e^{-\beta H} | q' \rangle.$$

Finally, we have for operator A

$$\langle A \rangle = \frac{\int dq dq' \rho(q, q'; \beta) \langle q | A | q' \rangle}{\int dq \rho(q, q; \beta)}.$$

For density matrix operator we can write expression

$$e^{-(\beta_1+\beta_2)H} = e^{-\beta_1 H} e^{-\beta_2 H}$$

and the same in coordinate representation

$$\rho(q_1, q_3; \beta_1 + \beta_2) = \int dq_2 \rho(q_1, q_2; \beta_1) \rho(q_2, q_3; \beta_2).$$

Applied this property N_t times

$$e^{-\beta H} = (e^{-\tau H})^{N_t},$$

where $\tau = \beta/N_t$. And in coordinate representation

$$\rho(q_0, q_N; \beta) = \int \dots \int dq_1 dq_2 \dots dq_{N-1} \rho(q_0, q_1; \tau) \rho(q_1, q_2; \tau) \dots \rho(q_{N-1}, q_N; \tau).$$

Operator of kinetic energy is diagonal in momentum representation and operator of potential energy is diagonal in coordinate representation. We can separate kinetic and potential energy if τ is small, so

$$e^{-\tau(T+V)+\frac{\tau^2}{2}[T,V]} = e^{-\tau T} e^{-\tau V}.$$

And if $\tau \rightarrow 0$

$$e^{-\tau(T+V)} \approx e^{-\tau T} e^{-\tau V}.$$

$$\rho(q_0, q_2; \tau) \approx \int dq_1 \langle q_0 | e^{-\tau T} | q_1 \rangle \langle q_1 | e^{-\tau V} | q_2 \rangle.$$

Potential energy is diagonal in position representation, so

$$\langle q_1 | e^{-\tau V} | q_2 \rangle = e^{-\tau V(q_1)} \delta(q_2 - q_1).$$

Using the expression $\int |p\rangle \frac{dp}{2\pi} \langle p| = 1$ we obtain

$$\langle q_0 | e^{-\tau T} | q_1 \rangle = \int dp dp' \delta(p - p') \langle q_0 | p \rangle \langle p' | q_1 \rangle e^{-T(p)\tau}.$$

Taking into account $\langle q | p \rangle = e^{-iqp}$, we obtain

$$\langle q_0 | e^{-\tau T} | q_1 \rangle = \int \frac{dp}{2\pi} e^{-T(p)\tau - ip(q_0 - q_1)}.$$

So to build path integral we must take this integral over momentum. Let's consider this integral in general case or, in other words, with general relativistic kinetic energy. We can calculate integral over momentum with this $T(p)$

$$\begin{aligned} \langle q_0 | e^{-\tau T} | q_1 \rangle &= \frac{m\tau}{\pi \sqrt{\tau^2 + (q_1 - q_0)^2}} K_1(m\sqrt{\tau^2 + (q_1 - q_0)^2}) = \\ &= \frac{m}{\pi \sqrt{1 + \left(\frac{q_1 - q_0}{\tau}\right)^2}} K_1(m\tau \sqrt{1 + \left(\frac{q_1 - q_0}{\tau}\right)^2}). \end{aligned}$$

where $K_1(*)$ is modified Bessel function of the first order. The general expression for matrix element is the following

$$\rho(q'', q'; \tau) = \langle q'' | e^{-\tau(T(p)+V(q))} | q' \rangle = \frac{m}{\pi \sqrt{1 + \left(\frac{q''-q'}{\tau}\right)^2}} K_1 \left[m\tau \sqrt{1 + \left(\frac{q''-q'}{\tau}\right)^2} \right] e^{-\tau V(q')}. \quad (16)$$

4 Path Integral Monte-Carlo Metropolis Algorithm

For Path Integral Monte-Carlo Metropolis algorithm we should know a part of the density matrix which corresponds to fixed point q_i . Discussion about this method and all proofs one can find in [7]. Using (16) we can write

$$\pi(q_i) = \frac{m^2 K_1 \left[m\tau \sqrt{1 + \left(\frac{q_i - q_{i-1}}{\tau}\right)^2} \right] K_1 \left[m\tau \sqrt{1 + \left(\frac{q_{i+1} - q_i}{\tau}\right)^2} \right]}{\pi^2 \sqrt{1 + \left(\frac{q_i - q_{i-1}}{\tau}\right)^2} \sqrt{1 + \left(\frac{q_{i+1} - q_i}{\tau}\right)^2}} e^{-\tau V(q_i)}.$$

So to calculate path integral we construct Markov chain which has equilibrium state for fixed q_i proportional to $\pi(q_i)$. Transition probability for this Markov chain satisfies equation

$$\int dq_i \pi(q_i) P(q_i \rightarrow q'_i) = \pi(q'_i).$$

We want to obtain $\pi(q)$ as limit of Markov chain, so we require the detailed balance

$$\pi(q_i) P(q_i \rightarrow q'_i) = \pi(q'_i) P(q'_i \rightarrow q_i).$$

In Metropolis algorithm we can split transition probability

$$P(q_i \rightarrow q'_i) = T(q_i \rightarrow q'_i) A(q_i \rightarrow q'_i),$$

where $T(q_i \rightarrow q'_i)$ is sampling distribution and $A(q_i \rightarrow q'_i)$ is acceptance probability

$$A(q_i \rightarrow q'_i) = \min \left[1, \frac{T(q'_i \rightarrow q_i) \pi(q'_i)}{T(q_i \rightarrow q'_i) \pi(q_i)} \right].$$

If we know density matrix in position representation, we can calculate expressions for average of any observables. Using (16) we can obtain the average of kinetic energy in general relativistic case (see [8]),

$$\langle T(p) \rangle = \left\langle \frac{m\tau}{\sqrt{\tau^2 + (\Delta q)^2}} \frac{K_0(m\sqrt{\tau^2 + (\Delta q)^2})}{K_1(m\sqrt{\tau^2 + (\Delta q)^2})} + \frac{\tau^2 - (\Delta q)^2}{\tau(\tau^2 + (\Delta q)^2)} \right\rangle. \quad (17)$$

Average of potential energy

$$\langle V(q) \rangle = \left\langle \frac{1}{2} m \omega^2 q_i^2 \right\rangle. \quad (18)$$

Full energy of ground state

$$\langle E(p, q) \rangle = \langle T(p) + V(q) \rangle.$$

Probability density

$$\rho(q) = |\psi(q)|^2 = \frac{1}{N\Delta q} \sum_{\text{all paths}} \theta(\Delta q - |q - q_i|), \quad (19)$$

where N - all simulation points. Correlation function

$$\langle q(t)q(t + n\tau) \rangle = \langle q_i q_{i+n} \rangle. \quad (20)$$

We have expressions for generating Markov chain and for calculating observables. Now we can compare results obtained by Monte-Carlo simulations and theretical predictions.

4.1 Non-relativistic limit

In this part we compare results obtained by PIMC program for $m \gg \omega$ case with theoretical predictions for harmonic oscillator. It is important to find proper values for the program because the quality of the results depends on them. Taking into account features of PIMC Metropolis algoritihm it is necessary to reach the limit of Markov chain and desired level of errors to compare results with analytical expressions. Designations to be used in this paper are the following: N_p - count of paths to be generated, N_s - count of sweeps for paths generation, N_t - count of time slices, τ - time step, N - count of attempts to change any q_i . Following data obtained at this parameters of program $N_p = 1000$, $N_s = 5000$, $N_t = 100$, $\tau = 0.1$, $N = 10$.

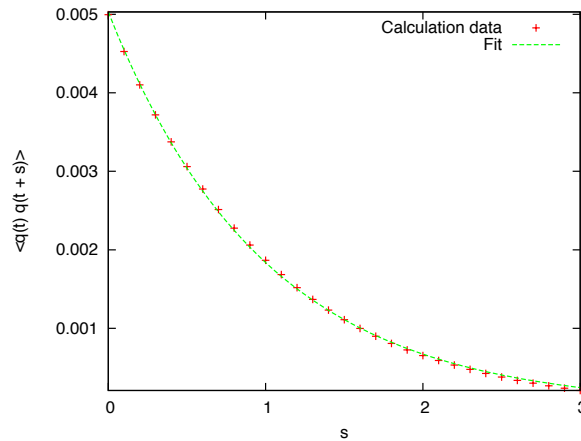


Figure 1: Correlation function for $m = 100$, $\omega = 1$.

For correlation function we have good agreement with theoretical expression (9) (see Fig. 1). Fit with function is the following

$$\langle q(t)q(t + s) \rangle = a \exp(-b|s|)$$

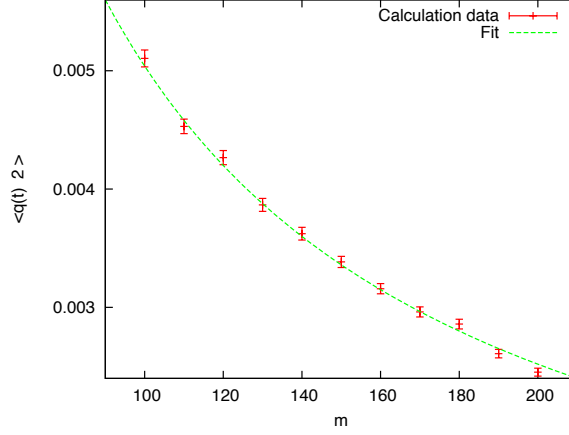


Figure 2: Dependence of $\langle q^2(t) \rangle$ on mass for $\omega = 1$.

where obtained values are $a = 1.006 \pm 0.004$ and $b = (503.0 \pm 1.4) \times 10^{-5}$. We know these values for harmonic oscillator $a = m\omega = 1$ and $b = 1/(2m\omega) = 500 \times 10^{-5}$.

Let's consider the comparison of results for $\langle q^2(t) \rangle$ (see Fig. 2). Fit with function is the following

$$\langle q^2(t) \rangle = \frac{a}{m}$$

where for a we obtained $a = 0.5040 \pm 0.0022$, and for harmonic oscillator $a = 1/(2\omega) = 0.5$.

Let's consider results of PIMC program for energy, we have analytical expressions (8) (see Fig. 3).

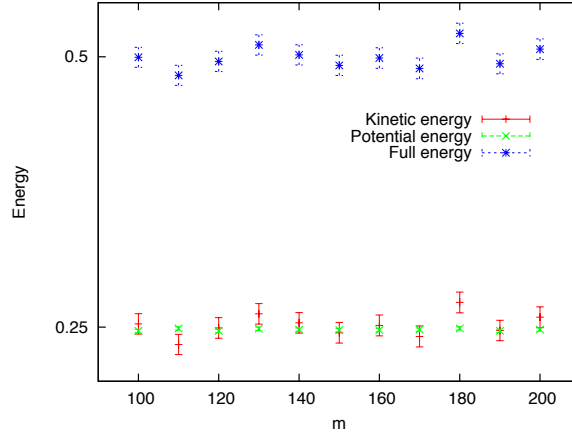


Figure 3: Dependence of Energy on mass for $\omega = 1$.

Fit with constant for this data

$$\langle T(p) \rangle = a$$

$$\langle V(q) \rangle = b$$

gives us $a = 0.251 \pm 0.003$, $b = 0.2476 \pm 0.0003$, where theoretical predictions are $a = b = \omega/4 = 0.25$.

We can compare density of probability with (7) (see Fig. 4).

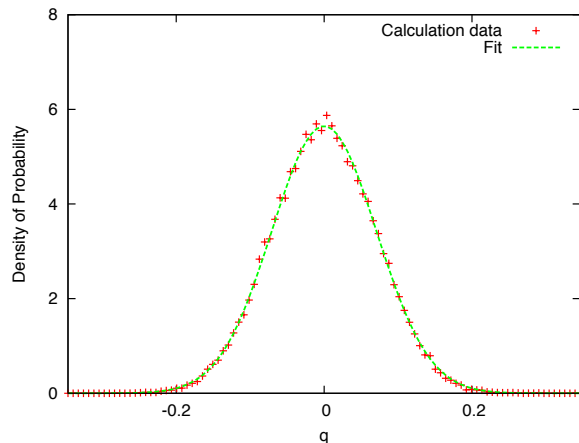


Figure 4: Dependence of Density of Probability $|\psi(q)|^2$ on q for $m = 100$, $\omega = 1$.

Fit with Gaussian function

$$\rho(q) = a \exp(-bq^2)$$

gives $a = 100.1 \pm 0.7$ and $b = 99.5 \pm 0.8$. We know that in non-relativistic limit $a = b = m\omega = 100$.

As we can see, we have an agreement with simple harmonic oscillator in the limit of $m \gg \omega$ or non-relativistic limit. Somewhere we have agreement with two or more standard deviations, it means that we should increase ratio of m and ω , but computer time of calculations for this case is longer.

4.2 Ultra-relativistic limit

In this section we compare results of PIMC Metropolis with $p^2 \gg m^2$ or $\omega \gg m$ limit. Parameters of program to be used for calculations are the following $N_p = 100$, $N_s = 5000$, $N_t = 1000$, $\tau = 0.01$, $N = 10$.

For correlation function we have (see Fig. 5).

Fit with exponential function

$$\langle q(t)q(t+s) \rangle = a \exp(-b|s|)$$

gives us $a = (536.5 \pm 1.8) \times 10^{-5}$ and $b = 10.60 \pm 0.05$. Although we did not find analytical expression for correlation function, there are a lot of arguments that should be the following

$$\langle q(t)q(t+s) \rangle = q^2(0)e^{-(\lambda_1 - \lambda_0)(m\omega^2)^{1/3}|s|}$$

where $\lambda_1(m\omega^2)^{1/3}$ is the next energy level of the ultra-relativistic oscillator, and $\lambda_1 = 2.338 \dots$. Theoretical values are $a = 0.539$ and energy gap $b = 10.47$. We have an agreement with theoretical expression for correlation function, so we can continue comparison of results.

Let's consider average of $q^2(t)$. We have an analytical expression

$$\langle q^2(t) \rangle = \frac{2\lambda_0}{3(m\omega^2)^{2/3}}$$

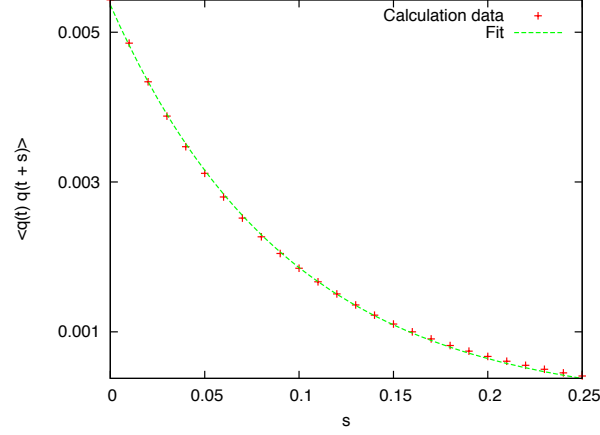


Figure 5: Dependence of Correlation function $\langle q(t)q(t+s) \rangle$ on $|s|$ for $m = 0.1$, $\omega = 100$.

and Monte-Carlo calculations give us following result (see Fig. 6)

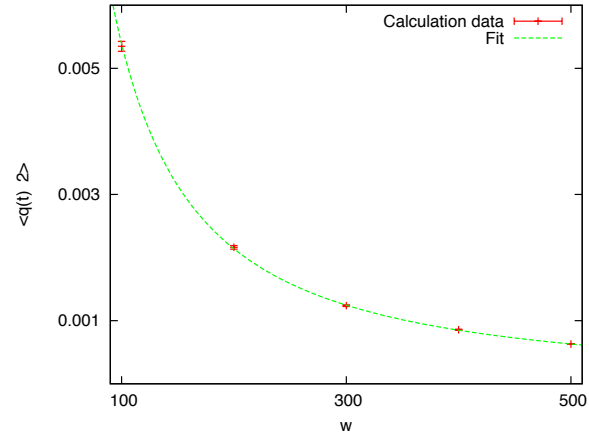


Figure 6: Dependence of $\langle q^2(t) \rangle$ on ω for $m = 0.1$.

Fit with function

$$\langle q^2(t) \rangle = \frac{2a}{3(0.1x^2)^{2/3}}$$

gives us $a = 0.8088 \pm 0.0027$, and theoretical prediction is $a = \lambda_0 = 0.8086 \dots$

Let us consider the calculations of energy for ultra-relativistic oscillator and compare them with analytical expressions (13), (14) (see Fig. 7).

Fit with functions

$$\langle T(p) \rangle = \frac{2}{3}a(m\omega^2)^{1/3},$$

$$\langle V(q) \rangle = \frac{1}{3}b(m\omega^2)^{1/3},$$

$$\langle E(p, q) \rangle = c(m\omega^2)^{1/3}$$

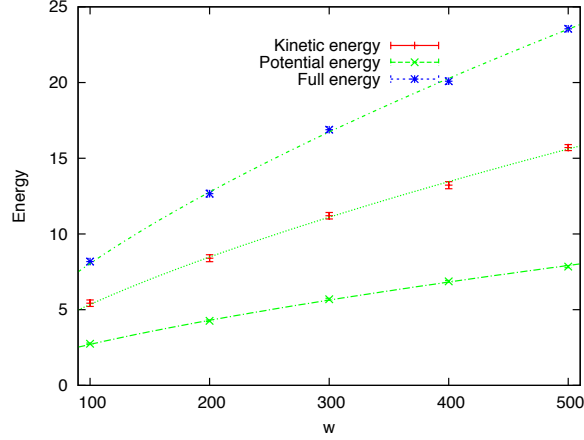


Figure 7: Dependence of Energy on ω for $m = 0.1$.

gives the following values $a = 0.801 \pm 0.004$, $b = 0.812 \pm 0.004$ and $c = 0.804 \pm 0.003$. Theoretical values are $a = b = c = \lambda_0 = 0.8086 \dots$

At the end of this section we compare Monte-Carlo calculations of density of probability with theoretical prediction (12) (see Fig. 8).

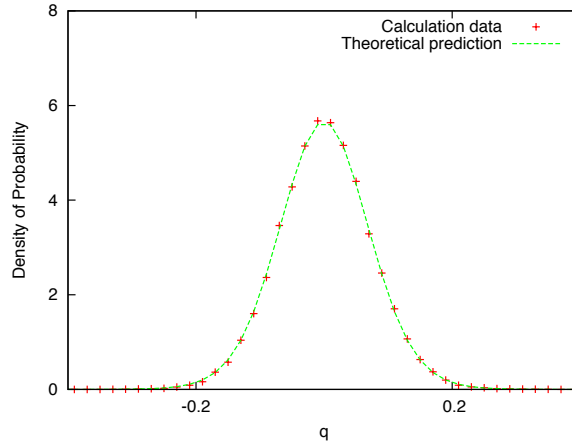


Figure 8: Dependence of Density of Probability on q for $m = 0.1$ and $\omega = 100$.

As a result, relativistic oscillator has a perfect agreement in ultra-relativistic limit with observables to be obtained from the following hamiltonian function

$$H \approx |p| + \frac{1}{2}m\omega^2 q^2.$$

5 Conclusion

The main goal of our work is to construct relativistic generalization of the PIMC method. This method we plan to use for investigation of the properties of the relativistic quantum medias with instantaneous interactions between the particles. Last fact gives us possibility

to avoid the problem with correctness of the many-body quantum-mechanical interaction. Of course, there are many interesting applications one can find in Relativistic Quantum Chemistry and Condensed Matter Physics.

To test our approach we study simple one-dimensional system with quadratic external potential - relativistic harmonic oscillator. This system gives us the possibility of testing our approach because relativistic harmonic oscillator can be studied by using Schrodinger equation in momentum space. The comparison of the results of these two approaches has shown that our relativistic generalization of PIMC method can be used for investigation of quantum systems which contain the relativistic particles. It is very essential to emphasize that in ultra-relativistic some special considerations are needed for solving the problem of thermalization of configuration.

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